Simulation of thermoelastic stresses with physical properties of refractory materials under the effect of thermal loads

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Abstract:

In this paper we propose the simulation of transient temperature field through the wall of a tubular combustion chamber, and the characterization of the thermal expansion, the thermoelastic stresses and strains with the physical properties of refractory materials. We simulate the tubular combustion chamber as a cylinder, where the geometry and physical properties of the material are known. It's the titanium alloy Ti-Nb-4.9 26.6.Al. The mathematical model is based on solving the heat equation in its general form (Transitional in three dimensions), coupled with laws of thermoelastic behavior. The finite differences method is used for the discretization of the differential equations with the explicit scheme, and a structured mesh is made for the discretization of the cylindrical geometry.

Keywords: Thermoelastic stresses, Transient temperature field Simulation, refractory material, finite differences method.

1. Introduction

The temperature reached in the aeronautical combustion chambers exceeds the limit characteristics of thermal resistance of current materials; it's for this reason that the temperature at the end of combustion must be controlled. The thrust of the engine is directly related to the temperature of gas emissions. We conceive the importance of having materials resistant to high temperatures, which have good mechanical strength and corrosion resistance, and can supporting overheating without the risk of weakening before high stresses (creep), and finally, these materials can be elaborated without need for heat treatment.

2. Geometric model

A flame tube is used as a model of tubular combustion chamber. To simplify the study, we simulate the geometrical form such as a cylinder defined by its inner radius R1, external radius R2 and its length L. the simulation of transient temperature field (heat transfer) through the tube wall is made by using a refractory material with known physical properties such as conductivity and thermal diffusivity. And to determine the thermal expansion or thermoelastic strains and stresses, we must know the mechanical properties of refractory materials such as modulus of elasticity (Young's modulus) and Poisson's coefficient. For the implementation of the mathematical model that governs the problem, a structured mesh in radial coordinates is developed for the discretization of the physical domain (Fig. 1a and 1b).

3. Radial heat transfer modeling

The mathematical model is based on the general heat equation in cylindrical coordinate system as follows[1]

$$\frac{1}{r}\frac{\partial}{\partial r}\left(k_1 r\frac{\partial T}{\partial r}\right)+\frac{1}{r^2}\frac{\partial}{\partial \theta}\left(k_2\frac{\partial T}{\partial \theta}\right)+\frac{\partial}{\partial z}\left(k_3\frac{\partial T}{\partial z}\right)+\dot{q}=\rho c\frac{\partial T}{\partial t} \tag{1}$$

ρ: Density *(kg / m³)*, C: specific heat *(kJ / kg.K) and* $\dot{q}$: heat flux *(W)*.

Equation (1) can be simplified by taking into account the following assumptions:

- ✓ Isotropic medium: k1 = k2 = k3 =λ, Homogeneous medium λ=f (T) = constant

Where λ is the thermal conductivity of the material (W / m K).

$$\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}+\frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2}+\frac{\partial^2 T}{\partial z^2}+\frac{\dot{q}}{\lambda}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{2}$$

With α : thermal diffusivity (m² / s).

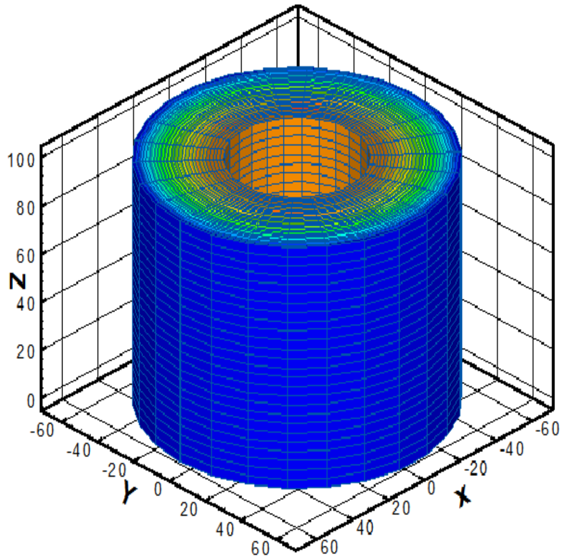

FIG. 1a- Overview of the computational domain (tubular combustion chamber)

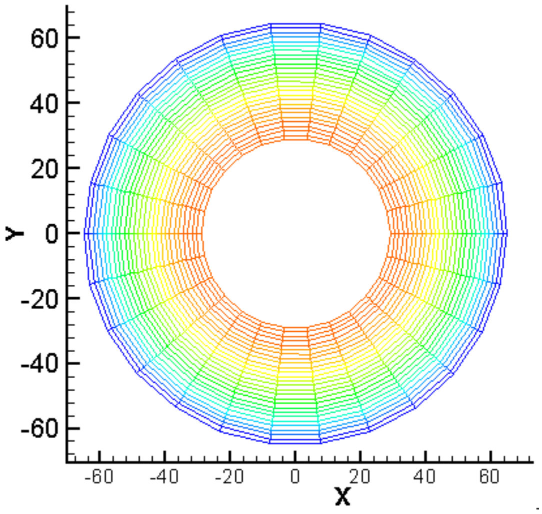

FIG.1b-Illustration mesh of the computational domain, Horizontal plane (top view)

- ✓ The temperature gradient versus (θ) is zero.
- ✓ It is assumed that the temperature gradient relative to Z is zero.

$$T=f(r,t)\Rightarrow\frac{\partial}{\partial\theta}=0\ \ et\ \ \frac{\partial}{\partial z}=0$$

So the equation (2) becomes [64]:

$$\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}+\frac{\dot{q}}{\lambda}=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3}$$

We set $\phi=\frac{\dot{q}}{\lambda}$, where ϕ is the heat source*(m K)*,

Equation (3) becomes [1,2,7] :

$$\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}+\phi=\frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{4}$$

4. Initial and boundary conditions

To close the problem, we must introduce the initial and boundary conditions, the system become:

$$\begin{cases}\dfrac{\partial^2 T}{\partial r^2}+\dfrac{1}{r}\dfrac{\partial T}{\partial r}+\phi=\dfrac{1}{\alpha}\dfrac{\partial T}{\partial t} & for\ \left(t>0\ and\ \ R_1<r<R_2\right)\\ \left.\dfrac{\partial T}{\partial r}\right|_{r=R_1}=0 & for\ \ \left(t>0\ and\ \ r=R_1\right). \quad (C1)\\ \left.\dfrac{\partial T}{\partial r}\right|_{r=R_2}+T(r,t)=1 & for\ \ \left(t>0\ and\ \ r=R_2\right). \quad (C2)\\ T(r,0)=\text{constant} & for\ \left(t=0\ and\ R_1<r<R_2\right). \quad (C3)\end{cases}$$

This boundary condition (C2) is a specification of a linear combination of the values of a temperature and the values of its derivative on the boundary of the domain. In addition, this equation is a general form of the boundary condition for convection–conduction equations. Here, the convective and conductive fluxes at the boundary sum to constant.

5. Discretization of the equations by the finite differences method

For the discretization of the equations, we used the finite differences method (explicit scheme) [2,7,8,11]:
Where i: subscript of space, k: subscript of time, r: radius and h: step of mesh.

$$r = \frac{dt}{h^3}\ ; \qquad r_i = (i-1)h$$

$$\left.\frac{\partial^2 T}{\partial r^2}\right|_{(i,k)} + \frac{1}{r}\left.\frac{\partial T}{\partial r}\right|_{(i,k)} + \phi = \frac{1}{\alpha}\left.\frac{\partial T}{\partial t}\right|_{(i,k)} \tag{5}$$

$$\left(\frac{1}{h^2}\right)\left(T_{i-1}^k - 2T_i^k + T_{i+1}^k\right) + \left(\frac{1}{r_1}\right)\frac{T_{i+1}^k - T_i^k}{2h} + \phi = \frac{1}{\alpha}\frac{T_i^{k+1} - T_i^k}{dt} \tag{6}$$

For i=2, n-1

$$T_i^{k+1} = \left(\alpha.r - \frac{\alpha.r}{2(i-1)}\right)T_{i-1}^k + (1-2r.\alpha)T_i^k + \left(\alpha.r + \frac{\alpha.r}{2(i-1)}\right)T_{i+1}^k + \alpha.\phi.dt \tag{7}$$

For i=1

The indetermination $\frac{1}{r}\frac{dT}{dr} \rightarrow 0$ could be lifted using l'Hôpital's rule: $\lim_{r\to 0}\frac{1}{r}\frac{dT}{dr} = \lim_{r\to 0}\frac{d^2T}{dr^2}$

So the equation (5) becomes around r = 0:

$$2\left(\frac{d^2T}{dr^2}\right)_{(1,k)} + \phi = \frac{1}{\alpha}\left(\frac{dT}{dt}\right)_{(1,k)} \tag{8}$$

$$\left(\frac{2}{h^2}\right)\left(T_0^k - 2T_1^k + T_2^k\right) + \phi = \left(\frac{1}{\alpha}\right)\frac{T_1^{k+1} - T_1^k}{dt} \tag{9}$$

$T_0^k \rightarrow$ To remove this fictitious point, we use the boundary condition $\left.\frac{\partial T}{\partial r}\right|_{r=R_1} = 0$ at r=R_1

$$\frac{T_2^k - T_0^k}{2h} = 0 \Rightarrow T_0^k = T_2^k$$

At i=1, $$T_1^{k+1} = (1-4r\alpha)T_1^k + 4r\alpha T_2^k + \alpha.\phi.dt \tag{10}$$

At r=R_2 (i=n):

$$T_n^{k+1} = \left(\alpha.r - \frac{\alpha.r}{2(n-1)}\right)T_{1-1}^k + (1-2.r.\alpha)T_n^k + \left(\alpha.r + \frac{\alpha.r}{2(n-1)}\right)T_{n+1}^k + \alpha.\phi.dt \tag{11}$$

$T_{n+1}^k \rightarrow$ To remove this fictitious point, we use the boundary condition $T_{n+1}^k \rightarrow \left.\frac{\partial T}{\partial n}\right|_{(n,k)} + T_{(n,k)} = 1$

$$\frac{T_{n+1}^k - T_{n-1}^k}{2h} + T_n^k = 1 \Rightarrow T_{n+1}^k = T_{n-1}^k - 2.h.T_n^k + 2.h \tag{12}$$

$$T_{n+1}^k = 2r.\alpha + \left(1 - 2\alpha.r - 2\alpha.r.h - \frac{2.\alpha.r.h}{2(n-1)}\right).T_n^k + (2r.\alpha.h)\left(1 + \frac{1}{2(n-1)}\right) + \alpha.\phi.dt \tag{13}$$

Finally we have a complete system to solve explicitly, it's formed of equations: (10, 7 and 13). Remains the choice of the material with the introduction of its physical properties, conductivity and thermal diffusivity.

6. Determination of thermoelastic behavior of the combustion chamber

Materials are often submitted to thermal loads which have the effect of expanding the volumes of structures. Thermal deformations are directly proportional to the temperature variation according to the coefficient of thermal expansion.

$$\underline{\varepsilon}^{th} = \beta.\Delta T\ \underline{I} \tag{14}$$

According to Amiot [3], if we set L_0 the initial length of a solid and T_0 its initial temperature, then its linear expansion is given by:

$$\Delta L = L - L_0 = \beta.L_0 \Delta T$$

From where:

$$L = L_0\left(1+\beta.\Delta T\right) \tag{15}$$

For the two-dimensional case,

$$S = S_0\left(1+\beta.\Delta T\right)^2 \tag{16}$$

With S_0. Initial section, S: Final section and $\Delta T = T - T_0$.

When the structure is not mechanically connected to the outside, then this field will not generate heat distortion constraints and the temperature field is linear in structure. Otherwise, if the structure is mechanically connected to the outside (called dilation upset), then constraints will be generated in the solid[4,7,9,10].

In the isotropic linear elastic case, we obtain a relation between the strains and stresses in the form:

$$\underline{\varepsilon} = \frac{1+\nu}{E}\underline{\sigma} + \left(\beta\,\Delta T - \frac{\nu}{E} tr\left(\underline{\sigma}\right)\right)\underline{I} \tag{17}$$

The inversion of this relationship gives us the law of behavior called "thermoelastic" of the material:

$$\underline{\sigma} = \frac{E}{1+\nu} + \left(\underline{\varepsilon}\frac{\nu}{1-2\nu} tr\left(\underline{\varepsilon}\right)\underline{I}\right) - \frac{E}{1-2\nu}\beta\ \Delta T\ \underline{I} \tag{18}$$

With $\underline{\sigma}, \underline{\varepsilon}, \underline{I}$: are respectively stress, deformation and identity tensor.

E: modulus of elasticity or (Young's modulus) of the material.

ν, β : Poisson and thermal expansion coefficient respectively.

According to CROS & FENG [5], if we consider that the material is isotropic and taking into account the constraints of thermal origin in one direction, we can write:

$$\sigma_{th} = -\frac{E\beta\Delta \mathrm{T}}{1-b\nu} \quad where \begin{cases} b=1 \ in\ plane\ constraints \\ b=2\ in\ plane\ deformations \end{cases} \tag{19}$$

7. Choice of material

The material used in our simulation is a superalloy of titanium base, its physical and mechanical properties are given in Table 1.

Table 1 Physical and mechanical properties of Ti-Nb-4.9 26.6.Al [6,7].

Titanum alloy	T(k)	E(GPa) Longitudinal modulus of elasticity	G(GPa) Transversal modulus of elasticity	ν Poisson coefficient	β(100) K^-1 Thermal expansion	λ : (W/m K) Thermal conductivity
Ti-26.6.Al-4.9 Nb	300-1156	134.47-0.0489T	53.56-0.018T	0.257- .00004T	$9.77\ 10^{-6}+4.46\ 10^{-9}$.T	21

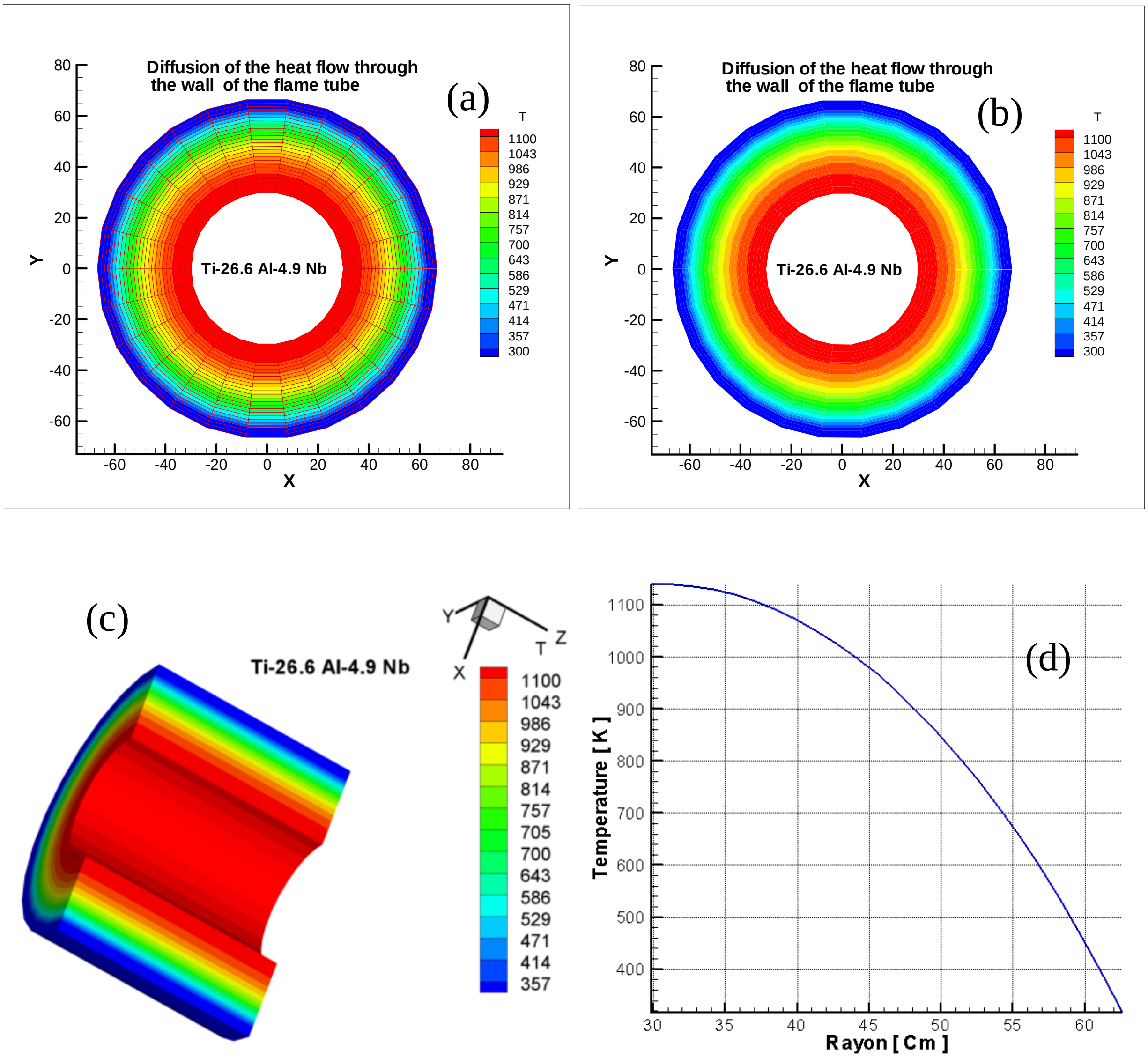

FIG.2. Radial distribution of the field of temperature for Titanium alloy (Ti-26.6Al4.9Nb) **)[7,9]**.

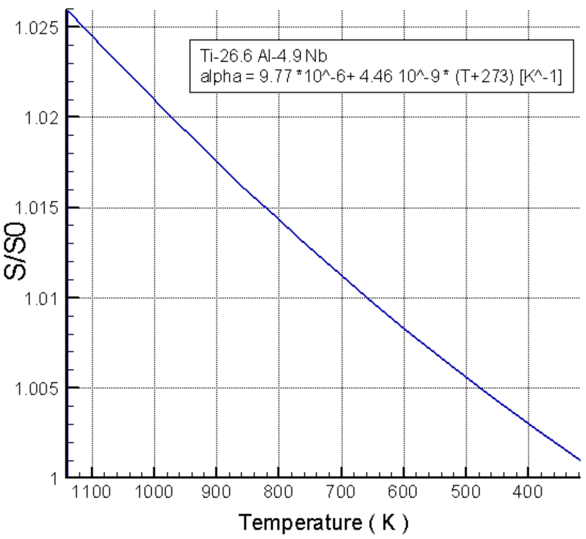

FIG.3 expansion of the section under the thermal effect.

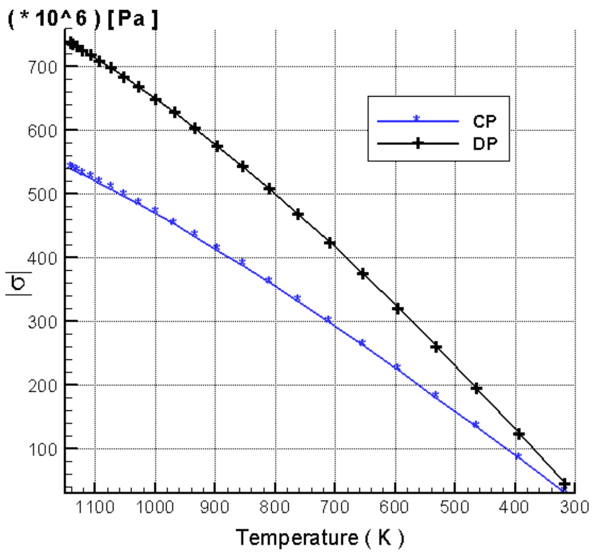

FIG.4 Variation of thermal stress under the effect of heat.
CP: Plane Constraints; DP: Plane Deformations

8. Results and comments

The radial distribution of the temperature field is shown in Figure 2, which illustrates the transfer of heat by conduction through the structure of the combustion chamber. In Figure 2. (A) and 2. (B), shows a view from above, with and without mesh of the combustion chamber, also illustrates the distribution of the temperature field in the form of a spectrum, which diffuses from the inner wall to the outer. A legend accompanies each figure shows the values of each level of the spectrum. The Figure A.2-c is a section in perspective to describe the same phenomenon. In Figure 1-d we characterize the parabolic variation of temperature versus the radius of the structure of combustion chamber.

The combustion chamber is submitted to thermal loads which have the effect of expanding structures. Thermal deformations are directly proportional to the variation of the temperature and thermal expansion coefficient β. FIG 3 illustrates the radial expansion of the combustion chamber under the effect of temperature. This is reflected in the variation of the sections ratio S/S0 according to the temperature. We note that the cylinder section ratio is to the maximum at high temperature and it comes at one for low temperatures, which means that the expansion is zero at low temperatures. In Figure 4 we present the variation of the thermal stress due to temperature, we observe also that the stress is to the maximum for high temperatures and becomes weak for low temperature.

9. Conclusion

In this study, we simulated a tubular combustion chamber as a cylinder with the geometry and physical properties of the material are known, a numerical calculation program is developed for the characterization and simulation of the transient temperature field (heat transfer) through the wall, as well as thermal expansion, thermoelastic stresses and strains based on the physical properties of the refractory material. It is concluded that the distribution of temperature fields through the wall is parabolic, the thermal deformation is directly proportional to the variation of the temperature and thermal expansion coefficient, and also the thermal stresses are highest for high temperatures and become minimum for low temperatures.

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